

H_2^+ in a strong magnetic field described via a solvable model

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Abstract. We consider the hydrogen molecular ion H_2^+ in the presence of a strong homogeneous magnetic field. In this regime, the effective Hamiltonian is almost one dimensional with a potential energy which looks like a sum of two Dirac delta functions. This model is solvable, but not close enough to our exact Hamiltonian for relevant strength of the magnetic field. However we show that the correct values of the equilibrium distance as well as the binding energy of the ground state of the ion, can be obtained when incorporating perturbative corrections up to second order. Finally, we show that He_2^{3+} exists for sufficiently large magnetic fields.

1. Introduction

Since the discovery of strong magnetic fields in astronomical objects, e.g., in the surface of neutron stars, the behaviour of atoms and molecules in these media has become a subject of wide interest. Also, high-magnetic-field conditions can be mimicked in some semiconductors where a small effective electron mass m_* and a large dielectric constant ϵ reduce the Coulomb force relative to the magnetic force [11]. For a review and references see [21, 23, 11, 22]. In particular, the hydrogen molecular ion H_2^+ , has been studied under the influence of a strong magnetic field in the last 25 years, see e.g., [2, 10, 12, 18, 16, 17, 8, 7, 19, 20, 25, 27, 26] for some references, using variational and numerical techniques. This system, as the simplest molecule in nature, can exhibit a qualitative behaviour of the internuclear separation as a function of the magnetic field that could have applications to the study of more complex molecular systems.

We consider H_2^+ , in a constant magnetic field. We use the Born-Oppenheimer approximation, with $-e$ and m_e the electric charge and the mass of the electron, respectively. In Gaussian units the Hamiltonian is given by

$$H = \frac{1}{2m_e} \left(\vec{p} + \frac{e}{c} \vec{A} \right)^2 - eV + \frac{e^2}{R} + H_{\text{spin}}, \quad (1)$$

where

$$V = e \left(\frac{1}{|\vec{r} - \frac{R}{2}\hat{z}|} + \frac{1}{|\vec{r} + \frac{R}{2}\hat{z}|} \right) \quad (2)$$

is the Coulomb potential due to the nuclei, and R the internuclear separation. Here $H_{\text{spin}} = \frac{e}{m_e c} \vec{S} \cdot \vec{B}$ and \vec{A} is the magnetic vector potential.

In this static situation it is convenient to use the Coulomb gauge $\vec{\nabla} \cdot \vec{A} = 0$, and the choice $\vec{A} = -\frac{1}{2} \vec{B} \times \vec{r}$. The magnetic field \vec{B} is taken parallel to the unit vector \hat{z} of the nuclear axis, which is the energetically most favorable situation [26, 12].

The criterium to define the strong magnetic field regime is to ask for a gap between Landau levels bigger than an energy of the order of the ionization energy of the hydrogen atom. This means

$$\hbar\omega_0 = \frac{e^2}{a_0} = 27.2 \text{ eV} = 1 \text{ Hartree}, \quad (3)$$

where $\omega_0 = eB_0/m_e c = 4.13 \times 10^{16} \text{ seg}^{-1}$ is the cyclotron frequency and $a_0 = \hbar^2/m_e e^2 = 0.53 \text{ \AA}$, the Bohr radius. That gives us the threshold value of B ,

$$B_0 = \frac{m_e^2 e^3 c}{\hbar^3} = 2.35 \times 10^9 \text{ G}. \quad (4)$$

The Hamiltonian can be written as

$$H = \hbar\omega_0 \left[\frac{a_0^2 \vec{p}^2}{\hbar^2} \frac{1}{2} - \frac{1}{2} \left(\frac{B}{B_0} \right) \frac{L_z}{\hbar} + \frac{1}{8} \left(\frac{B}{B_0} \right)^2 \frac{(x^2 + y^2)}{a_0^2} - a_0 V + \left(\frac{B}{B_0} \right) \frac{S_z}{\hbar} + \frac{a_0}{R} \right], \quad (5)$$

where $L_z = xp_y - yp_x$. Choosing atomic units, i.e., $m_e = \hbar = e = 1$, the Hamiltonian reads

$$H = \frac{p_z^2}{2} + H_{\text{osc}} - \frac{B}{2} L_z + B S_z - V + \frac{1}{R}, \quad (6)$$

where

$$H_{\text{osc}} = \frac{p_x^2 + p_y^2}{2} + \frac{B^2}{8}(x^2 + y^2). \quad (7)$$

In this system of units, the magnetic field is measured in units of $B_0 = c \approx 137$, the energy in units of $\hbar\omega_0 = 1$ Hartree = 27.2 [eV] and the separation R in units of $a_0 = 0.53$ [Å]. Moreover, using cylindrical coordinates (i.e., $x = \rho \cos \varphi$, $y = \rho \sin \varphi$ and $z = z$),

$$V(z, \rho) = \frac{1}{((z - \frac{R}{2})^2 + \rho^2)^{\frac{1}{2}}} + \frac{1}{((z + \frac{R}{2})^2 + \rho^2)^{\frac{1}{2}}}. \quad (8)$$

2. Spectral decomposition

In order to diagonalize H , we use that $[H, L_z] = [H, S_z] = [L_z, S_z] = 0$ and the spectral decompositions

$$L_z = \bigoplus_{m \in \mathbb{Z}} m \Pi^{(m)} \quad \text{and} \quad S_z = \bigoplus_{s_z = \pm 1/2} s_z \Pi^{(s_z)} \quad (9)$$

to get a diagonal matrix $H = \bigoplus H^{(m, s_z)} \Pi^{(m)} \otimes \Pi^{(s_z)}$ where

$$H^{(m, s_z)} = \frac{p_z^2}{2} + H_{\text{osc}}^{(m)} - \frac{B}{2}m + Bs_z - V + \frac{1}{R}, \quad (10)$$

and $H_{\text{osc}}^{(m)} = \frac{B}{2} \bigoplus_{n=0}^{\infty} (|m| + 2n + 1) \Pi_n^{(m)}$. Here $\Pi_n^{(m)}$ denotes the projector of the n^{th} eigenvalue of $H_{\text{osc}}^{(m)}$.

The ground state belongs to $s_z = -\frac{1}{2}$ in the spin sector and to $m = 0$ in the L_z sector, assuming that the result of [1] applies also to H_2^+ . So, we take the term

$$H^{(0, -\frac{1}{2})} = h^{(0, -\frac{1}{2})} + \frac{1}{R}, \quad (11)$$

where $h^{(0, -\frac{1}{2})} = \frac{p_z^2}{2} + H_{\text{osc}}^{(0)} - \frac{B}{2} - V$. Using the projectors of the spectral decomposition of $H_{\text{osc}}^{(0)}$ we can write $h^{(0, -\frac{1}{2})}$ in a matrix form as follows

$$h^{(0, -\frac{1}{2})} = \begin{pmatrix} \Pi_{\text{eff}} h^{(0, -\frac{1}{2})} \Pi_{\text{eff}} & \Pi_{\text{eff}} h^{(0, -\frac{1}{2})} \Pi_{\perp} \\ \Pi_{\perp} h^{(0, -\frac{1}{2})} \Pi_{\text{eff}} & \Pi_{\perp} h^{(0, -\frac{1}{2})} \Pi_{\perp} \end{pmatrix}, \quad (12)$$

where $\Pi_{\text{eff}} = \Pi_0^{(0)}$ and $\Pi_{\perp} = 1 - \Pi_{\text{eff}}$, and $\Pi_0^{(0)}$ the projector over the lowest Landau level. The “effective” part of our Hamiltonian, which is the physically relevant, $h_{\text{eff}} = \Pi_{\text{eff}} h^{(0, -\frac{1}{2})} \Pi_{\text{eff}}$, can be written as

$$h_{\text{eff}} = \frac{p_z^2}{2} - V_{\text{eff}} \quad (13)$$

with

$$V_{\text{eff}}(z) = B \int_0^{\infty} e^{-\frac{B\rho^2}{2}} V(z, \rho) \rho d\rho, \quad (14)$$

since Π_{eff} projects onto the wave function

$$\psi_0^{(0)}(\rho) = \sqrt{\frac{B}{2\pi}} e^{-\frac{B\rho^2}{4}}. \quad (15)$$

Making the change of variable, $u = \frac{B\rho^2}{2}$ we get

$$V_{\text{eff}}(z) = \int_0^\infty e^{-u} \tilde{V}(z, u) du \quad (16)$$

with

$$\tilde{V}(z, u) = \frac{1}{\left((z - \frac{R}{2})^2 + \frac{2u}{B}\right)^{\frac{1}{2}}} + \frac{1}{\left((z + \frac{R}{2})^2 + \frac{2u}{B}\right)^{\frac{1}{2}}}. \quad (17)$$

In the sequel we present some necessary mathematical results which will appear in full elsewhere [3]. Let U_L be the unitary implementation of the scaling $z \rightarrow z/L$ and define the scaled matrix as $h_L = \frac{1}{L^2} U_L h^{(0, -\frac{1}{2})} U_L^{-1}$. Its singular part reads

$$h_{\text{eff}}^L = \frac{p_z^2}{2} - \frac{1}{L^2} V_L, \quad (18)$$

where $V_L = V_L^- + V_L^+$ and

$$V_L^\mp(z) = \int_0^\infty \frac{e^{-u}}{\left(\frac{1}{L^2} \left(z \mp \frac{RL}{2}\right)^2 + \frac{2u}{B}\right)^{\frac{1}{2}}} du. \quad (19)$$

If we consider the resolvents $r_L = (h_L - \xi)^{-1}$ and $r_\delta = (h_\delta - \xi)^{-1} \otimes \Pi_{\text{eff}} \oplus 0$ where

$$h_\delta = \frac{p_z^2}{2} - \delta \left(z - \frac{RL}{2} \right) - \delta \left(z + \frac{RL}{2} \right), \quad (20)$$

we can show that [3]

$$\|r_L - r_{\text{eff}}^L\| \leq \frac{C_1}{\sqrt{B}} \quad \text{and} \quad \|r_{\text{eff}}^L - r_\delta\| \leq \frac{C_2}{L} \quad (21)$$

with $r_{\text{eff}}^L = (h_{\text{eff}}^L - \xi)^{-1}$, the resolvent of h_{eff}^L , and C_1 and C_2 are some positive constants. The appropriate scaling law for L in terms of the magnetic field is given by $L = L(B) = 2W(\frac{\sqrt{B}}{2})$, where $W(x)$ denotes the Lambert function (for more information about this function see [5]). This relationship between L and the magnetic field B is the correct scaling law to insure the convergence of the resolvents of the two different models which follows from the proof of the key theorem in [3]. Such a resolvent estimate implies, in particular, that the ground state of h_L , our scaled Hamiltonian, is asymptotic to e_0 , the ground state of h_δ , when the magnetic field tends to infinity.

3. Perturbation theory

In what follows, we will compute the ground state of h_{eff}^L perturbatively from the asymptotic model h_δ .

The ground state energy, e_0 , of h_δ is given by

$$e_0 = -\frac{\alpha_0^2}{2} \quad \text{with} \quad \alpha_0 = 1 + \frac{W(2ae^{-2a})}{2a}, \quad (22)$$

where $a = RL/2$. Here α_0 is the solution of the equation $\alpha_0 = 1 + e^{-2a\alpha_0}$, which can be expressed as (22), in terms of the Lambert function W .

Since the Hamiltonians h_L and h_δ are invariant under parity and since the ground state is even, it is convenient to work from here on in $L^2(\mathbf{R}^+)$. This being the case, the ground state of h_δ in $L^2(\mathbf{R}^+)$ reads,

$$\psi_0(z) = \begin{cases} A_1 e^{-\alpha_0 z} & z > a \\ A_2 \cosh(\alpha_0 z) & z < a \end{cases}, \quad (23)$$

with $A_1 = \alpha_0 e^{2a\alpha_0} A_2/2$ and $A_2 = 2/\sqrt{2(2a + e^{2a\alpha_0})}$.

We set

$$\Delta V = h_{\text{eff}}^L - h_\delta = \delta(z - a) - \frac{1}{L^2} V_L. \quad (24)$$

To second order in perturbation theory, the ground state energy of h_{eff}^L is given by [9]

$$e_2 = e_0 + \text{tr}(P_0 \Delta V P_0) - \text{tr}(P_0 \Delta V \hat{r}_\delta \Delta V P_0) \quad (25)$$

where P_0 is the projector over ψ_0 and \hat{r}_δ is the corresponding reduced resolvent.

The free kernel is given by

$$G_0(x, y; \xi) = \frac{1}{\sqrt{-2\xi}} \left(e^{-\sqrt{-2\xi}|x-y|} + e^{-\sqrt{-2\xi}(x+y)} \right) \quad (26)$$

and we use the notation $\partial_\xi G_0(x, y; \xi) \equiv \partial G_0(x, y; \xi)/\partial \xi$. Let $G_0(x, y)$ be the free kernel evaluated at $\xi = e_0$, and correspondingly we let $\partial_\xi G_0(x, y)$ be $\partial_\xi G_0(x, y; \xi)$ evaluated at $\xi = e_0$. Using this notation, the kernel of the reduced resolvent at $\xi = e_0 = -\alpha_0^2/2$ is given by

$$\hat{G}(x, y) = G_0(x, y) + \begin{pmatrix} G_0(x, a) & \partial_\xi G_0(x, a) \end{pmatrix} \begin{pmatrix} A_3 & A_4 \\ A_4 & 0 \end{pmatrix} \begin{pmatrix} G_0(a, y) \\ \partial_\xi G_0(a, y) \end{pmatrix} \quad (27)$$

with

$$A_3 = \frac{1}{2} \frac{\partial_\xi^2 G_0(a, a)}{(\partial_\xi G_0(a, a))^2}, \quad A_4 = \frac{-1}{\partial_\xi G_0(a, a)}. \quad (28)$$

Therefore, we can compute for each B and R the energy of the molecule H_2^+ in a magnetic field, now including the scaling and the repulsion energy, using the expression

$$E_2(B, R) = L^2(B) e_2(B, R) + \frac{1}{R}. \quad (29)$$

The minimum of $E_2(B, R)$ as a function of R , determines the equilibrium distance between the nuclei as well as the binding energy, which is defined as this minimum. We set $E_2 \equiv E_2(B, R_{eq})$, where R_{eq} denotes the equilibrium distance.

4. Numerical results

We have computed, with Mathematica [15], the equilibrium distance and binding energy of the H_2^+ molecule using second order perturbation theory, for a wide range of magnetic fields. Using the high level language of Mathematica, our program to compute $E_2(R)$ is simply a transcription in this language of the mathematical formula (25), (29) and (31). Simple and double integrals are made with the numerical integration of Mathematica using the Gauss-Kronrod method option. Plotting $R \rightarrow E_2(R)$ we are able to locate R_{eq} and finally to compute $E_2(R_{eq})$. In tables I, II, III and IV, we compare our results for the binding energy and internuclear separation, respectively, with those found by de Melo et al. [16] (using variational techniques), Le Guillou et al. [12], Lai et al. [10] and Heyl et al. [13], respectively. In figures 1 and 2 we plot the binding energy, and in figure 3 we plot the internuclear equilibrium distance, both against the natural scaling of these quantities, i.e., L^2 for the binding energy and L for the internuclear distance. Finally, in figure 4 we see that the product $R_{eq}L$ is monotonically decreasing as B increases.

5. Stability of homonuclear diatomic molecules with one electron

So far we have discussed the behavior of the ground state of H_2^+ for large magnetic fields. In this section we will consider homonuclear diatomic molecules with one electron but with nuclear charge not necessarily one. We are interested on the stability of these molecules as a function of Z and B . In particular, we are interested in determining the highest value of Z for which a diatomic molecule of this sort may exist, as a function of the strength of the magnetic field. We have not try to go beyond realistic values of B , i.e. $B \geq 10^{15}$. We will use the same model as the one discussed above but this time with nuclear charge Z . In order to take into account the explicit dependence of the model on Z we must change a to $a(Z) = ZRL/2$ and $V_L^\mp(z)$ to

$$V_L^\mp(z, Z) = \int_0^\infty \frac{e^{-u}}{\left(\frac{1}{L^2} \left(z \mp \frac{ZRL}{2}\right)^2 + \frac{2uZ^2}{B}\right)^{\frac{1}{2}}} du \quad (30)$$

and, correspondingly, the second order perturbation theory expression for the energy of the system is given by

$$E_2(B, R, Z) = Z^2 \left[L^2(B) e_2(B, R, Z) + \frac{1}{R} \right]. \quad (31)$$

Here e_2 is given, as before, by (25), but with the appropriate changes in ΔV .

In the case of zero magnetic field, it was shown numerically by Hogreve [14], that a homonuclear diatomic molecule with one electron exists as long as Z is below $Z_{crit} = 1.2367$. From our calculations here (see Table V below) we see that the magnetic field enhances the binding properties of this molecular ion. The maximum Z for which a homonuclear diatomic molecule with one electron exists, is a monotonically increasing function of B . Concerning our notation in Table V, below Z_c^{bs} we have a bound state

of the molecule. Between Z_c^{bs} and Z^{cr} we have only a local minimum, i.e., a resonance. Above Z^{cr} , we have no minimum for the potential energy curve $R \rightarrow E_2(B, R)$, see (29), at finite values of R .

6. Concluding remarks

Applying perturbation theory to a solvable model, we have computed the binding energy and the internuclear separation for the H_2^+ molecule in the presence of a strong magnetic field. Our results are in good agreement with those found in the literature for a wide range of the magnetic field. We also give the critical nuclear charge for the stability of diatomic molecules with one electron in a strong magnetic field. We remark that for magnetic fields about 10^{13} gauss, we can find a diatomic molecule with one electron with a nuclear charge $Z = 2$, which is a new atomic system. Finally, we note that one advantage of perturbation theory on variational methods is to give the possibility of computing numerically a window which contains the exact value of the ground state energy $E(R)$ of the effective Hamiltonian h_{eff} . In other words to produce lower bounds on $E(R)$ whereas variational methods are not good at that. Even using (21) we may compute these windows for the ground state energy of the complete Hamiltonian H . We hope to come back to this question in a further work.

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Table 1. Comparative table of data with those ones calculated by de Melo et al.[16] (with a \star).

B (Gauss)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq}^* (a.u)	$-E^*$ (Hartree)
1×10^{10}	1.494	1.49	1.232	1.42
5×10^{10}	0.813	2.92	0.736	2.77
1×10^{11}	0.632	3.84	0.604	3.64
5×10^{11}	0.364	6.97	0.351	6.59
1×10^{12}	0.291	8.86	0.285	8.38
5×10^{12}	0.182	14.90	0.179	14.08
1×10^{13}	0.148	18.35	0.149	17.32
5×10^{13}	0.099	28.76	0.104	26.90
1×10^{14}	0.084	34.40	0.085	31.86

Table 2. Comparative table of data with those ones calculated by Guillou et al.[12] (with a \star).

B (Gauss)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq}^* (a.u)	$-E^*$ (Hartree)
1.175×10^{10}	1.403	1.59	1.358	1.54
2.35×10^{10}	1.073	2.14	1.038	2.06
3.525×10^{10}	0.923	2.53	0.893	2.43
4.7×10^{10}	0.830	2.84	0.803	2.73
5.875×10^{10}	0.766	3.11	0.740	2.98
1.175×10^{11}	0.596	4.08	0.578	3.91
2.35×10^{11}	0.467	5.30	0.455	5.08
4.7×10^{11}	0.371	6.82	0.362	6.54
7.05×10^{11}	0.325	7.86	0.318	7.55
1.175×10^{12}	0.276	9.36	0.271	9.01
2.35×10^{12}	0.224	11.75	0.221	11.35
4.7×10^{12}	0.183	14.62	0.181	14.17

Table 3. Comparative table of data with those ones calculated by Lai et al.[10] (with a \star).

B (Gauss)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq}^* (a.u)	$-E^*$ (Hartree)
1×10^{11}	0.632	3.84	0.61	3.67
5×10^{11}	0.364	6.97	0.35	6.69
1×10^{12}	0.291	8.86	0.280	8.53
2×10^{12}	0.235	11.16	0.230	10.78
5×10^{12}	0.180	14.90	0.180	14.46
8×10^{12}	0.158	17.18	0.15	16.71
1×10^{13}	0.148	18.35	0.15	17.88
1×10^{14}	0.084	34.40	0.085	33.83
5×10^{14}	0.060	50.60	0.060	50.07

Table 4. Comparative table of data with those ones calculated by Heyl et al.[13] (with a \star).

B (Gauss)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq}^* (a.u.)	$-E^*$ (Hartree)
9.4×10^{12}	0.151	18.02	-	17.52
2.35×10^{13}	0.119	23.43	-	22.89
4.7×10^{13}	0.100	28.29	-	27.69
9.4×10^{13}	0.085	33.87	-	33.28
2.35×10^{14}	0.070	42.44	-	41.73
4.7×10^{14}	0.061	49.89	-	49.14

Table 5. Data of the stability study of the system

Z=1			Z=1.2		Z=1.4	
B (Gauss)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq} (a.u.)	$-E_2$ (Hartree)
1×10^{10}	1.494	1.49	1.718	1.71		
1×10^{11}	0.632	3.84	0.712	4.51	0.810	5.19
1×10^{12}	0.291	8.86	0.318	10.58	0.353	12.27
1×10^{13}	0.148	18.36	0.157	22.23	0.168	25.98
1×10^{14}	0.084	34.40	0.087	42.33	0.090	50.05

Z=1.6			Z=1.8		Z=2	
B (Gauss)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq} (a.u.)	$-E_2$ (Hartree)
1×10^{12}	0.400	13.99	0.445	15.78		
1×10^{13}	0.183	29.67	0.202	33.39	0.227	37.26
1×10^{14}	0.095	57.55	0.101	64.88	0.108	72.14

Z=2.2			Z=2.4	
B (Gauss)	R_{eq} (a.u.)	$-E_2$ (Hartree)	R_{eq} (a.u.)	$-E_2$ (Hartree)
1×10^{14}	0.118	79.44	0.131	86.98

Table 6. Upper bounds to the critical nuclei charge of stability of the molecule given by our model.

B (Gauss)	Z_c^{bs}	Z^{cr}
1×10^{10}	< 1.32	< 1.58
1×10^{11}	< 1.55	< 2.05
1×10^{12}	< 1.80	< 2.60
1×10^{13}	< 2.10	< 3.10
1×10^{14}	< 2.43	< 3.50

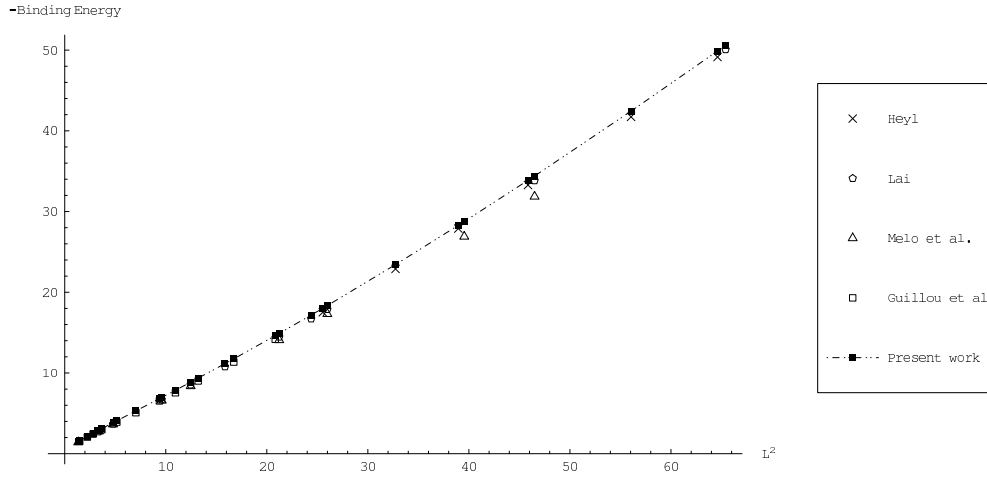


Figure 1. Comparison of the binding energies for all magnetic field values. The binding energy is plotted in atomic units. The adimensional scaling parameter L is calculated as $L = 2W(\frac{1}{2}\sqrt{\frac{B}{B_0}})$ and therefore is independent of system of units chosen for the magnetic field.

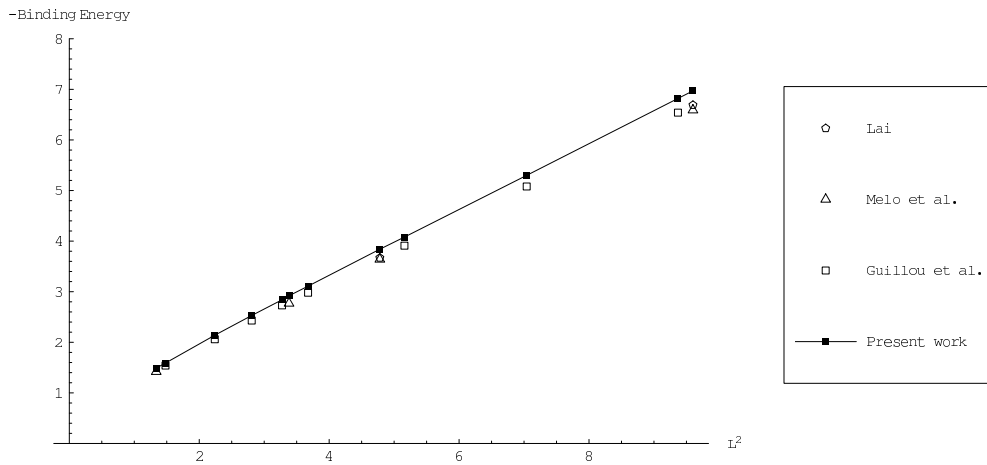


Figure 2. Detail of the figure 1

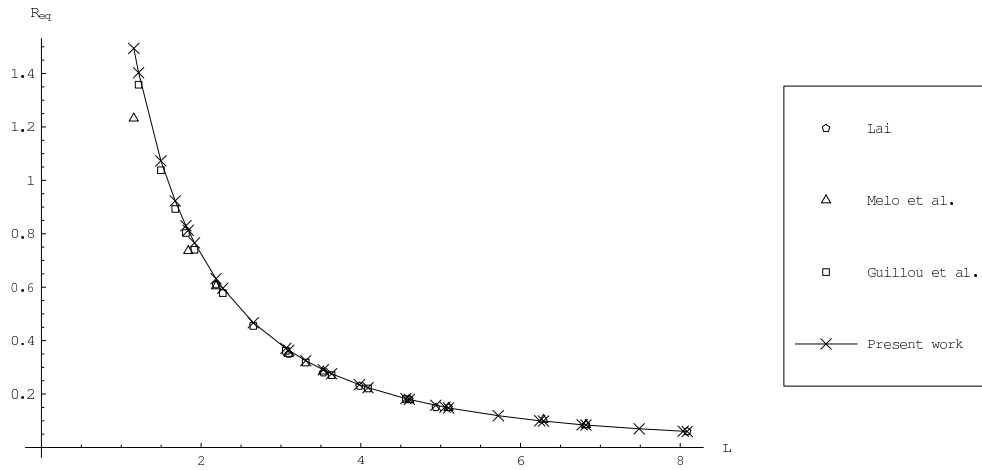


Figure 3. Comparison of the equilibrium internuclear distance, which is plotted in atomic units.

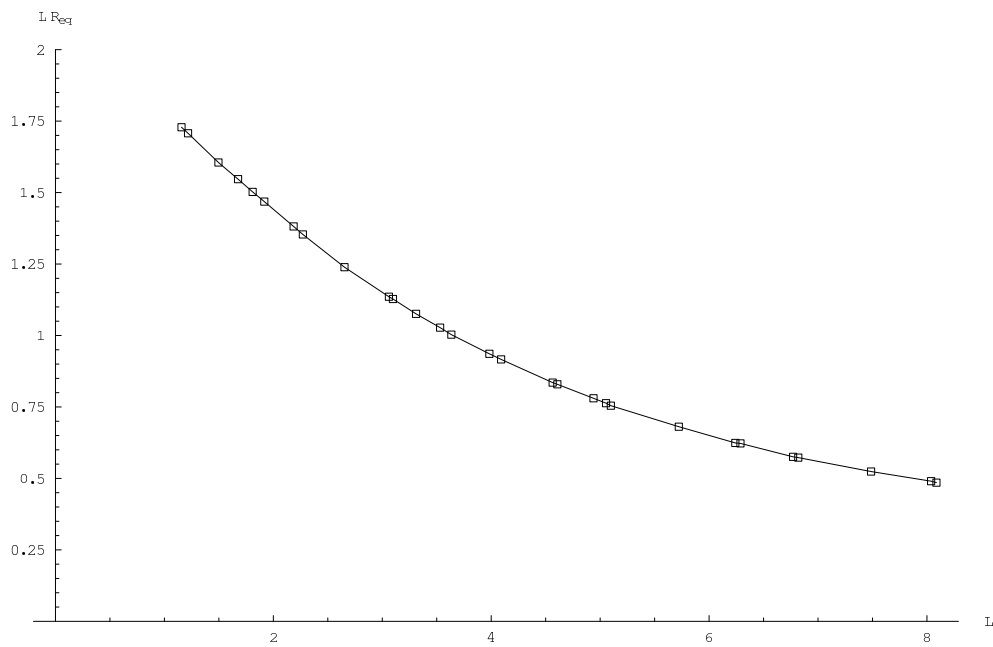


Figure 4. Behaviour of the product of R_{eq} L